

# CAUCHY-BORN RULE AND SPIN DENSITY WAVE FOR THE SPIN-POLARIZED THOMAS-FERMI-DIRAC-VON WEIZSÄCKER MODEL

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**ABSTRACT.** The electronic structure (electron charges and spins) of a perfect crystal under external magnetic field is analyzed using the spin-polarized Thomas-Fermi-Dirac-von Weizsäcker model. An extension of the classical Cauchy-Born rule for crystal lattices is established for the electronic structure under sharp stability conditions on charge density wave and spin density wave. A Landau-Lifshitz type micromagnetic energy functional is derived.

## 1. INTRODUCTION

The present paper is the fourth of a series of papers that are devoted to the study of the electronic structure of smoothly deformed crystals or crystals in an external field, by analyzing various quantum mechanics models at different levels of complexity, including the Kohn-Sham density functional theory, Thomas-Fermi type of models and tight-binding models. Our overall objective is to establish the microscopic foundation of the continuum theories of solids, such as the nonlinear elasticity theory and the theory of magnetic materials, in terms of quantum mechanics and to examine the boundary where the continuum theories break down.

In previous work [5–7], we have studied the nonlinear tight-binding model and the Kohn-Sham density functional theory, and established their continuum limits for smoothly deformed crystals. As a byproduct, we also derived macroscopic models for the piezoelectric effect of a material from many-body quantum theory. In the present work, we will focus on the magnetic properties of a material and the associated spin waves. We choose the spin-polarized Thomas-Fermi-Dirac-von Weizsäcker (TFDW) model as our starting point. This is a representative of a simplest version of the density functional theory in which the electronic structure is represented solely by the electron density instead of the wave functions as in the Kohn-Sham theory. As in the previous work, our reference point is the electronic structure of a perfect crystal, *i.e.* the equilibrium crystal lattice without external fields. The solution of the TFDW model we are interested in is a continuation of the solution

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for the unperturbed system. This works as long as certain stability conditions are satisfied. One main objective is to identify these stability conditions, with emphasis on the stability of spin density waves (magnons). The overall strategy is similar to the one in the previous paper [6] and [5].

Another related work that we should mention is [1] where the Thomas-Fermi-von Weizsäcker model (without spin-polarization) was studied for smoothly deformed crystals. It was shown that in the continuum limit, the total energy of the system converges to a limiting value given by the extended Cauchy-Born construction. There, the stability condition is automatically satisfied since the model is convex. [4] extended this kind of results to the tight-binding models. The strategy in the current series of papers is quite different from those in [1] or [4]. Here our emphasis is on the stability conditions.

Throughout this paper, we use the notation  $\lesssim$  for inequalities up to an absolute constant:  $f \lesssim g$  if  $f \leq Cg$  where  $C$  is an absolute constant. Sometimes, it is more convenient to explicitly use  $C$  to denote the constant, which might change from line to line. When it is necessary to specify the dependence of the constant on parameters, we will use the notation  $C(a, b)$  to indicate that the constant depends on parameters  $a$  and  $b$ .

Standard notations are used for function spaces like  $L^p$ ,  $H^k$  and  $W^{k,p}$  so on. We also need function spaces for periodic functions. Let  $\mathbb{L} \subset \mathbb{R}^3$  be a lattice with unit cell  $\Gamma$ . Denote the reciprocal lattice as  $\mathbb{L}^*$  and its unit cell (the first Brillouin zone) as  $\Gamma^*$ . For a given  $n \in \mathbb{N}$ , we define

$$(1.1) \quad L_n^p = \{f \in \mathcal{S}'(\mathbb{R}^3) \mid \tau_R f = f, \forall R \in n\mathbb{L}; \int_{n\Gamma} |f|^p dx < \infty\},$$

with norm given by

$$(1.2) \quad \|f\|_{L_n^p} = \left( n^{-3} \int_{n\Gamma} |f|^p dx \right)^{1/p},$$

and similarly for  $L_n^\infty$ . Here  $\tau_R$  is the translational operator with translation vector  $R$ ,  $(\tau_R f)(x) = f(x - R)$ . The periodic Sobolev space  $H_n^k$  is defined similarly

$$(1.3) \quad H_n^k = \{f \in \mathcal{S}'(\mathbb{R}^3) \mid \tau_R f = f, \forall R \in n\mathbb{L}; f \in H^k(n\Gamma)\}, \quad k \in \mathbb{Z}_+$$

with norm

$$(1.4) \quad \|f\|_{H_n^k} = \sum_{|\alpha| \leq k} \|\partial^\alpha f\|_{L_n^2},$$

where  $\alpha$  denotes a multi-index and  $\partial^\alpha$  the corresponding partial derivative. Moreover, we also define the periodic homogeneous Sobolev space with index  $-1$  as

$$(1.5) \quad \dot{H}^{-1}(n\Gamma) = \{f \in \mathcal{S}'(\mathbb{R}^3) \mid \tau_R f = f \forall R \in n\mathbb{L}, \sum_{k \in \mathbb{L}^*/n} \frac{1}{|k|^2} |\widehat{f}(k)|^2 < \infty\}.$$

Here,  $\{\widehat{f}(k)\}$  denotes the Fourier coefficients of the  $n\Gamma$ -periodic function  $f$

$$(1.6) \quad \widehat{f}(k) = (2\pi)^{-3/2} \int_{n\Gamma} f(x) e^{-ik \cdot x} dx.$$

The space  $\dot{H}^{-1}(n\Gamma)$  is a Hilbert space with inner product

$$(1.7) \quad \langle f, g \rangle_{\dot{H}^{-1}(n\Gamma)} = 4\pi \sum_{k \in \mathbb{L}^*/n} \frac{1}{|k|^2} \overline{\widehat{f}(k)} \widehat{g}(k).$$

For Banach spaces  $X$  and  $Y$ ,  $\mathcal{L}(X, Y)$  denotes the class of bounded linear operators from  $X$  to  $Y$  and  $\|\cdot\|_{\mathcal{L}(X, Y)}$  denotes the operator norm. When  $X = Y$ , we use  $\mathcal{L}(X) = \mathcal{L}(X, X)$ .

## 2. SPIN-POLARIZED THOMAS-FERMI-DIRAC-VON WEIZSÄCKER MODEL

We consider the spin-polarized Thomas-Fermi-Dirac-von Weizsäcker (TFDW) model. We will restrict ourselves to the collinear case, that is, we assume that the applied magnetic field is parallel to a fixed axis (with possibly varying amplitude). In the spin-polarized TFDW model, the electronic structure is characterized by the spin-up and spin-down densities, corresponding to the density of spin-up and spin-down electrons. Denote by  $\rho_+$  and  $\rho_-$  the spin-up and spin-down densities respectively, the energy of the system is given by

$$(2.1) \quad I^h(\rho_+, \rho_-) = \int \rho_+^{5/3} + \rho_-^{5/3} + |\nabla \sqrt{\rho_+}|^2 + |\nabla \sqrt{\rho_-}|^2 - \int \rho_+^{4/3} + \rho_-^{4/3} \\ + \frac{1}{2} D(\rho - \rho_b, \rho - \rho_b) - \int h m.$$

Here  $\rho = \rho_+ + \rho_-$  is the total charge density,  $m = \rho_+ - \rho_-$  is the spin density or magnetization density, and  $\rho_b$  is charge contribution from the nuclei and core electrons. The shorthand notation  $D(\cdot, \cdot)$  is defined as

$$D(f, g) = \iint \frac{f(x)g(y)}{|x - y|} dx dy.$$

Finally,  $h$  is the external magnetic field, which is a scalar, since we have assumed the collinearity.

The density satisfies the normalization constraint

$$(2.2) \quad \int \rho = \int \rho_b,$$

and the positivity constraint  $\rho_+, \rho_- \geq 0$ . To deal with the positivity constraint, it is often convenient to introduce the variables

$$\nu_+ = \sqrt{\rho_+}, \quad \nu_- = \sqrt{\rho_-}.$$

In terms of  $\nu_+$  and  $\nu_-$ , we have

$$(2.3) \quad I^h(\nu_+, \nu_-) = \int \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int \nu_+^{8/3} + \nu_-^{8/3} \\ + \frac{1}{2} D(\rho - \rho_b, \rho - \rho_b) - \int h m,$$

where

$$\rho = \nu_+^2 + \nu_-^2, \quad m = \nu_+^2 - \nu_-^2.$$

The energy is given by the variational problem

$$(2.4) \quad E^h = \inf_{\nu_{\pm} \in H^1(\mathbb{R}^3)} I^h(\nu_+, \nu_-)$$

with the normalization constraint (2.2). The Euler-Lagrange equation associated with the energy functional reads,

$$(2.5) \quad -\Delta \nu_+ + \frac{5}{3} \nu_+^{7/3} - \frac{4}{3} \nu_+^{5/3} + V \nu_+ - h \nu_+ = \lambda \nu_+;$$

$$(2.6) \quad -\Delta \nu_- + \frac{5}{3} \nu_-^{7/3} - \frac{4}{3} \nu_-^{5/3} + V \nu_- + h \nu_- = \lambda \nu_-;$$

$$(2.7) \quad -\Delta V = 4\pi(\rho - \rho_b),$$

where  $\lambda$  is a Lagrange multiplier corresponds to the normalization constraint.

In this work, we will consider the TFDW model for crystals with and without the external magnetic field. We denote  $\mathbb{L}$  the underlying Bravais lattice of the crystal and  $\Gamma$  the unit cell of the crystal. The charge background  $\rho_b$  is  $\Gamma$ -periodic and assumed to be smooth (in other words, we are taking a pseudo-potential approximation). When there is no external magnetic field, the electronic structure is characterized by the periodic-TFDW model, with energy functional

$$(2.8) \quad I_{\Gamma}^0(\nu_+, \nu_-) = \int_{\Gamma} \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int_{\Gamma} \nu_+^{8/3} + \nu_-^{8/3} \\ + \frac{1}{2} D_{\Gamma}(\rho - \rho_b, \rho - \rho_b),$$

where the periodic Coulomb interaction  $D_{\Gamma}$  is given by

$$D_{\Gamma}(f, g) = \langle f, g \rangle_{\dot{H}^{-1}(\Gamma)}.$$

The electronic structure is given by the variational problem

$$(2.9) \quad E_{\Gamma}^0 = \inf_{\nu_{\pm} \in H_{\Gamma}^1} I_{\Gamma}^0(\nu_+, \nu_-)$$

with the normalization constraint that

$$\int_{\Gamma} \nu_+^2 + \nu_-^2 = \int_{\Gamma} \rho_b = Z.$$

Here  $Z$  is some fixed integer.

The Euler-Lagrange equations associated with (2.9) are given by

$$(2.10) \quad -\Delta\nu_+ + \frac{5}{3}\nu_+^{7/3} - \frac{4}{3}\nu_+^{5/3} + V\nu_+ = 0;$$

$$(2.11) \quad -\Delta\nu_- + \frac{5}{3}\nu_-^{7/3} - \frac{4}{3}\nu_-^{5/3} + V\nu_- = 0;$$

$$(2.12) \quad -\Delta V = 4\pi(\rho - \rho_b).$$

The equations are defined on  $\Gamma$  with periodic boundary conditions. Note that we have absorbed the Lagrange multiplier into the potential  $V$ , as (2.12) only determines  $V$  up to a constant. The normalization constraint is also implicitly imposed as the solvability condition of (2.12).

It is easy to see that the minimum of the variational problem (2.9) is achieved and the minimizers satisfy the Euler-Lagrange equations. The minimizers might not be unique since the Dirac term  $(-\int \nu_+^{8/3} + \nu_-^{8/3})$  is concave. Let us take one of the minimizers, denoted as  $\nu_{+,\text{per}}$  and  $\nu_{-,\text{per}}$ , and let us denote the corresponding potential as  $V_{\text{per}}$  (with the Lagrange multiplier included). By standard elliptic regularity theory, it is easy to see that  $\nu_{\pm,\text{per}}, V_{\text{per}} \in C^\infty(\Gamma)$ . We extend them to the whole  $\mathbb{R}^3$  periodically. It is also straightforward to see that  $\nu_{\pm,\text{per}}$  are non-negative. It is possible that  $\nu_{-,\text{per}} \equiv 0$  is a minimizer (while the corresponding  $\nu_{+,\text{per}} > 0$ ). To exclude such cases, we will assume that there exists a positive constant  $C_\nu$  such that

$$(2.13) \quad \nu_{\pm,\text{per}}(x) \geq C_\nu, \quad x \in \Gamma.$$

We may also consider the energy functional defined on the supercell  $n\Gamma$  for  $n \in \mathbb{N}$ :

$$(2.14) \quad I_{n\Gamma}^0(\nu_+, \nu_-) = \int_{n\Gamma} \nu_+^{10/3} + \nu_-^{10/3} + |\nabla\nu_+|^2 + |\nabla\nu_-|^2 - \int_{n\Gamma} \nu_+^{8/3} + \nu_-^{8/3} \\ + \frac{1}{2}D_{n\Gamma}(\rho - \rho_b, \rho - \rho_b),$$

where

$$D_{n\Gamma}(f, g) = \langle f, g \rangle_{\dot{H}^{-1}(n\Gamma)}.$$

The corresponding Euler-Lagrange equations have the same form as (2.10)–(2.12) defined now on  $n\Gamma$  with periodic boundary conditions. The functions  $\nu_{\pm,\text{per}}, V_{\text{per}}$  (recall that we have extended them to  $\mathbb{R}^3$  periodically) still satisfy the Euler-Lagrange equation and hence are stationary points of the functional (2.14).

### 3. STABILITY ANALYSIS

**3.1. Stability of Electronic Structure.** For any  $n \in \mathbb{N}$ , let us define the linear operator  $\mathcal{L}$ , which is the linearization of the Euler-Lagrange equations (2.10)–(2.12) on the domain  $n\Gamma$ , given by

$$(3.1) \quad \mathcal{L} \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix} = \begin{pmatrix} \mathcal{L}_+ & 0 & \nu_+ \\ 0 & \mathcal{L}_- & \nu_- \\ \nu_+ & \nu_- & \frac{1}{8\pi}\Delta \end{pmatrix} \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix},$$

where the operators  $\mathcal{L}_\pm$  are given by

$$(3.2) \quad \mathcal{L}_\pm \omega = -\Delta \omega + \frac{35}{9} \nu_\pm^{4/3} \omega - \frac{20}{9} \nu_\pm^{2/3} \omega + V \omega.$$

**Proposition 3.1.** *Assume  $\nu_\pm, V \in W_n^{k,\infty}$ , for some  $k \in \mathbb{N}$ . Then  $\mathcal{L}$  is a bounded operator from  $(H_n^{k+2})^3$  to  $(H_n^k)^3$ ,*

$$\|\mathcal{L}\|_{\mathcal{L}((H_n^{k+2})^3, (H_n^k)^3)} \lesssim \|\nu_+\|_{W_n^{k,\infty}} + \|\nu_-\|_{W_n^{k,\infty}} + \|V\|_{W_n^{k,\infty}} + 1.$$

Moreover, if  $\nu_\pm, V \in L_n^\infty$ , then  $\mathcal{L}$  is a self-adjoint operator on the domain  $\mathcal{D}(\mathcal{L}) = (H_n^2)^3$ .

*Proof.* Denote

$$\begin{pmatrix} f_+ \\ f_- \\ g \end{pmatrix} \equiv \mathcal{L} \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix},$$

then we have

$$\begin{aligned} f_+ &= -\Delta \omega_+ + \frac{35}{9} \nu_+^{4/3} \omega_+ - \frac{20}{9} \nu_+^{2/3} \omega_+ + V \omega_+ + W \nu_+; \\ f_- &= -\Delta \omega_- + \frac{35}{9} \nu_-^{4/3} \omega_- - \frac{20}{9} \nu_-^{2/3} \omega_- + V \omega_- + W \nu_-; \\ g &= \frac{1}{8\pi} \Delta W + \nu_+ \omega_+ + \nu_- \omega_-. \end{aligned}$$

It follows that

$$\begin{aligned} \|f_+\|_{H_n^k} &\leq C(\|\nu_+\|_{W_n^{k,\infty}}, \|V\|_{W_n^{k,\infty}}) \|\omega_+\|_{H_n^{k+2}} + \|\nu_+\|_{W_n^{k,\infty}} \|W\|_{H_n^{k+2}}; \\ \|f_-\|_{H_n^k} &\leq C(\|\nu_-\|_{W_n^{k,\infty}}, \|V\|_{W_n^{k,\infty}}) \|\omega_-\|_{H_n^{k+2}} + \|\nu_-\|_{W_n^{k,\infty}} \|W\|_{H_n^{k+2}}; \\ \|g\|_{H_n^k} &\leq \frac{1}{8\pi} \|W\|_{H_n^{k+2}} + \|\nu_+\|_{W_n^{k,\infty}} \|\omega_+\|_{H_n^{k+2}} + \|\nu_-\|_{W_n^{k,\infty}} \|\omega_-\|_{H_n^{k+2}}. \end{aligned}$$

Hence,  $\mathcal{L}$  is bounded with the desired estimate on the operator norm.

The self-adjointness of  $\mathcal{L}$  is an easy consequence of the Kato-Rellich theorem [9], since  $\nu_\pm$  and  $V$  viewed as multiplicative operators on  $H_n^2$  are infinitesimally small with respect to the Laplacian operator.  $\square$

Consider specifically the case when  $\nu_\pm$  and  $V$  given by the unperturbed system:

$$(3.3) \quad \mathcal{L}_{\text{per}} = \begin{pmatrix} \mathcal{L}_{+, \text{per}} & 0 & \nu_{+, \text{per}} \\ 0 & \mathcal{L}_{-, \text{per}} & \nu_{-, \text{per}} \\ \nu_{+, \text{per}} & \nu_{-, \text{per}} & \frac{1}{8\pi} \Delta \end{pmatrix},$$

with  $\mathcal{L}_{\pm, \text{per}}$  defined by

$$(3.4) \quad \mathcal{L}_{\pm, \text{per}} \omega = -\Delta \omega + \frac{35}{9} \nu_{\pm, \text{per}}^{4/3} \omega - \frac{20}{9} \nu_{\pm, \text{per}}^{2/3} \omega + V_{\text{per}} \omega.$$

**Assumption A** (Stability of the electronic structure). There exists a constant  $M$  independent of  $n$ , such that for any  $n$ ,

$$\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^3)} \leq M,$$

or equivalently, since  $\mathcal{L}_{\text{per}}$  is self-adjoint

$$\text{dist}(0, \text{spec}(\mathcal{L}_{\text{per}})) \geq 1/M.$$

Under the stability assumption, we can actually obtain estimates of  $\mathcal{L}_{\text{per}}^{-1}$  acting on higher order Sobolev spaces. The following result is standard, we include the proof here for completeness.

**Proposition 3.2.** *Under Assumption A and assume  $\nu_{\pm}, V \in W_n^{k,\infty}$ , for some  $k \in \mathbb{N}$ . Then we have*

$$\|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^k)^3, (H_n^{k+2})^3)} \leq C(k)M.$$

*Proof.* Let us consider  $k = 0$  first. It suffices to prove the estimate

$$(3.5) \quad \|A\mathcal{L}_{\text{per}}^{-1}u\|_{(H_n^2)^3} \lesssim M\|u\|_{(L_n^2)^3},$$

for any  $u = (\omega_+, \omega_-, W) \in (L_n^2)^3$ , where  $A$  is the operator

$$A = \begin{pmatrix} -\Delta & & \\ & -\Delta & \\ & & \frac{1}{8\pi}\Delta \end{pmatrix}.$$

The left hand side of (3.5) equals to

$$\begin{pmatrix} -\Delta & & \\ & -\Delta & \\ & & \frac{1}{8\pi}\Delta \end{pmatrix} \mathcal{L}_{\text{per}}^{-1}u = u - \begin{pmatrix} F_+ & 0 & \nu_{+, \text{per}} \\ 0 & F_- & \nu_{-, \text{per}} \\ \nu_{+, \text{per}} & \nu_{-, \text{per}} & 0 \end{pmatrix} \mathcal{L}_{\text{per}}^{-1}u,$$

where

$$F_{\pm} = \frac{35}{9}\nu_{\pm, \text{per}}^{4/3} - \frac{20}{9}\nu_{\pm, \text{per}}^{2/3} + V_{\text{per}}.$$

Therefore,

$$\begin{aligned} \|A\mathcal{L}_{\text{per}}^{-1}u\|_{(L_n^2)^3} &\lesssim \|u\|_{(L_n^2)^3} + \max(\|F_{\pm}\|_{L_n^{\infty}}, \|\nu_{\pm, \text{per}}\|_{L_n^{\infty}}) \|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^3)} \|u\|_{(L_n^2)^3} \\ &\lesssim M\|u\|_{(L_n^2)^3}. \end{aligned}$$

Suppose the statement of the Proposition is proved for  $k \leq k_0$ , let us consider  $k = k_0 + 1$ . Since

$$\begin{aligned} \nabla \mathcal{L}_{\text{per}}^{-1} &= \mathcal{L}_{\text{per}}^{-1} \nabla + [\nabla, \mathcal{L}_{\text{per}}^{-1}] \\ &= \mathcal{L}_{\text{per}}^{-1} \nabla - \mathcal{L}_{\text{per}}^{-1} [\nabla, \mathcal{L}_{\text{per}}] \mathcal{L}_{\text{per}}^{-1}, \end{aligned}$$

it suffices to control

$$\|\mathcal{L}_{\text{per}}^{-1} [\nabla, \mathcal{L}_{\text{per}}] \mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^k)^3, (H_n^{k+1})^3)},$$

where  $\nabla = I_3 \nabla$  with  $I_3$  the  $3 \times 3$  identity matrix. Note that

$$\begin{aligned} \|\mathcal{L}_{\text{per}}^{-1}[\nabla, \mathcal{L}_{\text{per}}]\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^k)^3, (H_n^{k+1})^3)} &\leq \|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^{k-1})^3, (H_n^{k+1})^3)} \\ &\quad \times \|[\nabla, \mathcal{L}_{\text{per}}]\|_{\mathcal{L}((H_n^{k+1})^3, (H_n^{k-1})^3)} \|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^{k-1})^3, (H_n^{k+1})^3)}. \end{aligned}$$

By assumption, the Proposition holds for  $k-1 = k_0$ , hence it suffices to control the commutator  $[\nabla, \mathcal{L}_{\text{per}}]$ . An explicit calculation yields

$$[\nabla, \mathcal{L}_{\text{per}}] = \begin{pmatrix} \nabla F_+ & 0 & \nabla \nu_{+, \text{per}} \\ 0 & \nabla F_- & \nabla \nu_{-, \text{per}} \\ \nabla \nu_{+, \text{per}} & \nabla \nu_{-, \text{per}} & 0 \end{pmatrix},$$

and hence the bounds follow from the regularity assumptions on  $\nu_{\pm, \text{per}}$  and  $V_{\text{per}}$ . The proposition is proved.  $\square$

The Assumption A is stated in terms of the operator  $\mathcal{L}_{\text{per}}$  acting on a series of spaces  $(L_n^2)^3$ . Using the Bloch-Floquet decomposition (see [10] or [7] for an introduction), we may obtain an equivalent characterization of the stability assumption. Note that  $\mathcal{L}_{\text{per}}$  commutes with the translational operator with respect to the lattice  $\mathbb{L}$  since  $\nu_{\pm, \text{per}}$  and  $V_{\text{per}}$  are  $\Gamma$ -periodic. Denote  $\Gamma^*$  as the unit cell of the reciprocal lattice of  $\mathbb{L}$ , the Bloch-Floquet decomposition of  $\mathcal{L}_{\text{per}}$  is given by

$$(3.6) \quad \mathcal{L}_{\text{per}} = \oint_{\Gamma^*} \mathcal{L}_{\xi, \text{per}} d\xi.$$

Here for any  $\xi \in \Gamma^*$ ,  $\mathcal{L}_{\xi, \text{per}}$  is the operator

$$(3.7) \quad \mathcal{L}_{\xi, \text{per}} = \begin{pmatrix} \mathcal{L}_{+, \xi, \text{per}} & 0 & \nu_{+, \text{per}} \\ 0 & \mathcal{L}_{-, \xi, \text{per}} & \nu_{-, \text{per}} \\ \nu_{+, \text{per}} & \nu_{-, \text{per}} & \frac{1}{8\pi} \Delta_\xi \end{pmatrix},$$

with  $\mathcal{L}_{\pm, \xi, \text{per}}$  given by

$$(3.8) \quad \mathcal{L}_{\pm, \text{per}} \omega = -\Delta_\xi \omega + \frac{35}{9} \nu_{\pm, \text{per}}^{4/3} \omega - \frac{20}{9} \nu_{\pm, \text{per}}^{2/3} \omega + V_{\text{per}} \omega.$$

We also have for any  $\xi$ , the operator  $\mathcal{L}_{\xi, \text{per}}$  defined on the space  $(L_\xi^2)^3$ , where

$$L_\xi^2 = \{f \in L_{\text{loc}}^2(\mathbb{R}^3) \mid e^{i\xi \cdot x} f(x) \text{ } \Gamma\text{-periodic}\},$$

is self-adjoint [10].

Using Bloch-Floquet decomposition of  $\mathcal{L}_{\text{per}}$ , the stability assumption can also be formulated as

**Assumption A'.** There exists a constant  $M$ , such that for each  $\xi \in \Gamma^*$ ,

$$\|\mathcal{L}_{\xi, \text{per}}^{-1}\|_{(L_\xi^2)^3} \leq M.$$

The proof of the equivalence of Assumption A and Assumption A' is parallel to the corresponding results in [5, 6] and is standard from Bloch-Floquet theory; hence, we omit it here.



**3.2. Example of stability and instability.** Let us consider the jellium model as an example to understand better the stability assumptions. For the jellium model, the charge background is a constant function  $\rho_b(x) = \rho_0$ . Define  $\nu_0 = \frac{1}{2}\rho_0^{1/2}$ , a solution to the Euler-Lagrange equations are given by

$$\nu_+(x) = \nu_0, \quad \nu_-(x) = \nu_0, \quad V(x) = 0, \quad \lambda = \frac{5}{3}\nu_0^{4/3} - \frac{4}{3}\nu_0^{2/3}.$$

Therefore,

$$(3.9) \quad \mathcal{L}_+\omega = \mathcal{L}_-\omega = -\Delta\omega + \frac{20}{9}\nu_0^{4/3}\omega - \frac{8}{9}\nu_0^{2/3}\omega.$$

We use Fourier transform to analyze the operator  $\mathcal{L}$ .

$$(3.10) \quad \mathcal{L}_\xi = \begin{pmatrix} \xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} & 0 & \nu_0 \\ 0 & \xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} & \nu_0 \\ \nu_0 & \nu_0 & -\frac{1}{8\pi}\xi^2 \end{pmatrix}$$

One eigenvalue of the matrix is

$$(3.11) \quad \lambda_{\xi,1} = \xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3},$$

corresponds to the eigenvector  $(1, -1, 0)^T$ . The other two eigenvalues are given by

$$(3.12) \quad \lambda_{\xi,\pm} = \frac{1}{2} \left( \frac{8\pi-1}{8\pi}\xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} \right. \\ \left. \pm \sqrt{\left( \frac{8\pi+1}{8\pi}\xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} \right)^2 + 8\nu_0^2} \right).$$

Observe that these two eigenvalues correspond to action of  $\mathcal{L}_\xi$  on the subspace orthogonal to the vector  $(1, -1, 0)^T$ , and hence, the first two components are the same.

It is easy to see that  $\lambda_{\xi,1}$  becomes positive if  $\xi$  is sufficiently large. To prevent  $\lambda_{\xi,1}$  from changing sign when  $\xi$  is small, we need

$$\xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} > 0, \quad \forall \xi,$$

or equivalently

$$(3.13) \quad \nu_0 > \left(\frac{2}{5}\right)^{3/2}.$$

For the other two eigenvalues, we have

$$\lambda_{\xi,+}\lambda_{\xi,-} = -\frac{1}{8\pi}\xi^2 \left( \xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} \right) - \nu_0^2.$$

The product becomes negative when  $\xi$  is sufficiently large, and hence we have  $\lambda_{\xi,-} < 0$  and  $\lambda_{\xi,+} > 0$  for  $\xi$  sufficiently large. To make sure they are nonzero for every  $\xi$ , we need

$$-\frac{1}{8\pi}\xi^2 \left( \xi^2 + \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} \right) - \nu_0^2 < 0, \quad \forall \xi,$$

which is equivalent to the condition that

$$(3.14) \quad \frac{20}{9}\nu_0^{4/3} - \frac{8}{9}\nu_0^{2/3} > -8\sqrt{\pi}\nu_0.$$

This condition is weaker than (3.13).

Hence, (3.13) guarantees that the three eigenvalues do not change sign for all  $\xi$ , and hence the matrix  $\mathcal{L}_\xi$  is non-singular.

Let us remark that physically, the condition (3.13) corresponds to the stability of spin-density-wave, since  $\lambda_{k,1}$  corresponds to the eigenvector  $(1, -1, 0)^T$ , which increases (or decreases) the spin-up component, while decreases (or increases) the spin-down component, hence creates a spin-density-wave. On the other hand, the condition (3.14) corresponds to the stability of charge-density-wave, since the spin-up and spin-down components change together with the same amplitude. For the jellium case, since the condition (3.14) is implied by the condition (3.13), we observe that the spin-density-wave loses stability earlier than the charge-density-wave when the uniform background charge density is decreased.

#### 4. CAUCHY-BORN RULE

Let us first consider the case when the applied magnetic field is constant  $h(x) \equiv h$ , and consider the cell problem

$$(4.1) \quad I_\Gamma^h(\nu_+, \nu_-) = \int_\Gamma \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int_\Gamma \nu_+^{8/3} + \nu_-^{8/3} \\ + \frac{1}{2}D_\Gamma(\rho - \rho_b, \rho - \rho_b) - hm_{\text{tot}},$$

where the periodic Coulomb interaction  $D_\Gamma$  is given by

$$D_\Gamma(f, g) = \langle f, g \rangle_{\dot{H}^{-1}(\Gamma)},$$

and the total magnetization  $m_{\text{tot}}$  is given by

$$m_{\text{tot}} = \int_\Gamma \nu_+^2 - \nu_-^2.$$

Consider

$$(4.2) \quad E(h) = \inf_{\nu_+, \nu_-} I_\Gamma^h,$$

with the normalization constraint  $\int_\Gamma \rho = Z$ . The Euler-Lagrange equations are given by

$$(4.3) \quad -\Delta \nu_+ + \frac{5}{3}\nu_+^{7/3} - \frac{4}{3}\nu_+^{5/3} + (V - h)\nu_+ = 0;$$

$$(4.4) \quad -\Delta \nu_- + \frac{5}{3}\nu_-^{7/3} - \frac{4}{3}\nu_-^{5/3} + (V + h)\nu_- = 0;$$

$$(4.5) \quad -\Delta V = 4\pi(\rho - \rho_b);$$

in the unit cell  $\Gamma$ , where  $h$  is a constant. Let us denote the equations as

$$\mathcal{F}(u, h) = 0,$$

where  $u$  stands for the triple  $u = (\nu_+, \nu_-, V)$ .

The following theorem shows that the solution  $u$  exists provided the stability condition is satisfied and the constant applied magnetic field  $h$  is not too large.

**Theorem 1.** *Under Assumption A, there exist positive constants  $h_0$  and  $\delta$ , and a unique  $C^\infty$  map from  $[-h_0, h_0] \rightarrow (H_1^3)^3$ :  $h \mapsto u(\cdot; h)$ , such that  $\|u(\cdot; h) - u_{\text{per}}\|_{(H_1^3)^3} \leq \delta$  and*

$$\mathcal{F}(u(\cdot; h), h) = 0.$$

*Proof.* We use the implicit function theorem. Let  $u_{\text{per}}$  be the triple  $(\nu_{\pm, \text{per}}, V_{\text{per}})$ , we have

$$\mathcal{F}(u_{\text{per}}, 0) = 0.$$

Let  $\delta_1$  be a positive constant to be fixed, consider the neighborhood around  $u_{\text{per}}$ :

$$\mathcal{D} = \{u \mid \|u - u_{\text{per}}\|_{(H_1^3)^3} \leq \delta_1\}.$$

Denote  $u = (\nu_\pm, V)$ ; by Sobolev inequality, we have

$$\|\nu_\pm - \nu_{\pm, \text{per}}\|_{L_1^\infty} \lesssim \|\nu_\pm - \nu_{\pm, \text{per}}\|_{H_1^2} \leq \delta_1.$$

Take  $\delta_1$  sufficiently small such that  $\|\nu_\pm - \nu_{\pm, \text{per}}\|_{L_1^\infty} \leq C_\nu/2$ . Hence, for  $u \in \mathcal{D}$ , we have  $\nu_\pm \geq C_\nu/2 > 0$ . It is then easy to see that viewed as an operator from  $\mathcal{D} \times \mathbb{R}^3 \rightarrow (H_1^1)^3$ ,  $\mathcal{F}$  is  $C^\infty$ . Notice that

$$\left. \frac{\delta \mathcal{F}(u, h)}{\delta u} \right|_{u=u_{\text{per}}, h=0} = \mathcal{L}_{\text{per}}$$

has a bounded inverse from  $(H_1^1)^3$  to  $(H_1^3)^3$  due to the stability assumption and Proposition 3.2. Applying the implicit function theorem on  $\mathcal{F}$ , we arrive at the desired result.  $\square$

*Remark.* It is clear from the proof that we can consider solutions in spaces with higher regularity. The space  $(H_1^3)^3$  is chosen here for proving the main result in the next section.

We denote the solutions given by Theorem 1 as  $\nu_{+, \text{CB}}(\cdot; h)$  and  $\nu_{-, \text{CB}}(\cdot; h)$  respectively for the spin-up and spin-down components, and  $V_{\text{CB}}(\cdot; h)$  for the potential. Here  $h$  is a parameter and  $\nu_{\pm, \text{CB}}$  and  $V_{\text{CB}}$  are  $\Gamma$ -periodic.

For  $h \in [-h_0, h_0]$ , let  $\mathcal{L}_h$  be the linearized operator around  $u_{\text{CB}}(\cdot, h)$ :

$$(4.6) \quad \mathcal{L}_h = \left. \frac{\delta \mathcal{F}(u, h)}{\delta u} \right|_{u=u_{\text{CB}}(\cdot; h), h=h},$$

given by

$$(4.7) \quad \mathcal{L}_h \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix} = \begin{pmatrix} \mathcal{L}_{h,+} & 0 & \nu_{+, \text{CB}}(\cdot; h) \\ 0 & \mathcal{L}_{h,-} & \nu_{-, \text{CB}}(\cdot; h) \\ \nu_{+, \text{CB}}(\cdot; h) & \nu_{-, \text{CB}}(\cdot; h) & \frac{1}{8\pi} \Delta \end{pmatrix} \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix},$$

where the operators  $\mathcal{L}_{h,+}$  and  $\mathcal{L}_{h,-}$  are defined as

$$(4.8) \quad \mathcal{L}_{h,+}\omega = -\Delta\omega + \frac{35}{9}\nu_{+,CB}^{4/3}(x;h)\omega - \frac{20}{9}\nu_{+,CB}^{2/3}(x;h)\omega + (V_{CB}(x;h) - h)\omega;$$

$$(4.9) \quad \mathcal{L}_{h,-}\omega = -\Delta\omega + \frac{35}{9}\nu_{-,CB}^{4/3}(x;h)\omega - \frac{20}{9}\nu_{-,CB}^{2/3}(x;h)\omega + (V_{CB}(x;h) + h)\omega.$$

By Proposition 3.1 and using similar arguments as the proof of Proposition 3.2, we have

**Proposition 4.1.** *Under the same assumptions of Theorem 1,  $\mathcal{L}_h$  as an operator from  $(H_1^3)^3$  to  $(H_1^1)^3$  is invertible, and the norm of the inverse operator is uniformly bounded for  $h \in [-h_0, h_0]$ .*

Let us remark that Theorem 1 gives a map from  $h$  to the electronic structure  $(\nu_+, \nu_-)$  for the case when the external magnetic field is homogeneous. This is slightly different from the usual Cauchy-Born rule for crystals under deformation, where the strain is fixed – here  $h$ , the analog of stress, is fixed. One may consider the dual problem given by

$$\begin{aligned} \tilde{E}_{CB}(m) = \inf_{\nu_{\pm}: m_{\text{tot}}=m} \left\{ \int_{\Gamma} \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int_{\Gamma} \nu_+^{8/3} + \nu_-^{8/3} \right. \\ \left. + \frac{1}{2|\Gamma|} D_{\Gamma}(\rho - \rho_b, \rho - \rho_b) \right\}, \end{aligned}$$

where  $m_{\text{tot}} = \int_{\Gamma} \nu_+^2 - \nu_-^2$  is constrained to be equal to  $m$ . This can be viewed as a Legendre transform of

$$\begin{aligned} E_{CB}(h) = \inf_{\nu_{\pm}} \int_{\Gamma} \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int_{\Gamma} \nu_+^{8/3} + \nu_-^{8/3} \\ + \frac{1}{2|\Gamma|} D_{\Gamma}(\rho - \rho_b, \rho - \rho_b) - \frac{1}{|\Gamma|} h m_{\text{tot}}. \end{aligned}$$

The formulation in terms of the magnetization  $m$  may bear more similarity with the conventional Cauchy-Born rule for lattices.

## 5. MAIN RESULTS

We turn to the situation when the system is under (a macroscopically heterogeneous) external applied magnetic field. We will study the case when the applied potential is macroscopically smooth. The ratio of the lattice constant and the characteristic length of  $h$  will serve as a small parameter  $\varepsilon$ . Given a fixed  $\Gamma$ -periodic function  $h(\cdot)$ , two equivalent choices of scalings are possible: For any  $\varepsilon = 1/n$  a reciprocal of positive integer, we may study a perfect crystal with applied field  $h(\varepsilon x)$  in  $n\Gamma$  with periodic boundary condition; equivalently, we may rescale the system, so that the lattice constant becomes  $\varepsilon$  and study the rescaled system with applied field  $h(x)$  in  $\Gamma$  with periodic boundary condition. We call the former choice the atomic unit scaling, and the latter choice the  $\varepsilon$ -scaling. We will use atomic unit

scaling for most part of the paper, however,  $\varepsilon$ -scaling is more convenient and is used for the two-scale analysis in Section 6.1.

Under the influence of the external field, the electronic structure of the system is determined by minimizing the energy functional.

$$(5.1) \quad I_n^h(\nu_+, \nu_-) = \int_{n\Gamma} \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int_{n\Gamma} \nu_+^{8/3} + \nu_-^{8/3} \\ + \frac{1}{2} D_n(\rho - \rho_b, \rho - \rho_b) - \int_{n\Gamma} h(\varepsilon x) m,$$

where  $D_n$  is the Coulomb interaction

$$D_n(f, g) = \langle f, g \rangle_{\dot{H}^{-1}(n\Gamma)},$$

and the density  $\rho$  and the spin density  $m$  are given by

$$\rho = \nu_+^2 + \nu_-^2, \quad m = \nu_+^2 - \nu_-^2.$$

The functional (5.1) is optimized under the normalization constraint on the electron density

$$(5.2) \quad n^{-3} \int_{n\Gamma} \rho = n^{-3} \int_{n\Gamma} \nu_+^2 + \nu_-^2 = Z.$$

The Euler-Lagrange equations associated with (5.1) are given by

$$(5.3) \quad -\Delta \nu_+ + \frac{5}{3} \nu_+^{7/3} - \frac{4}{3} \nu_+^{5/3} + (V - h(\varepsilon x)) \nu_+ = 0;$$

$$(5.4) \quad -\Delta \nu_- + \frac{5}{3} \nu_-^{7/3} - \frac{4}{3} \nu_-^{5/3} + (V + h(\varepsilon x)) \nu_- = 0;$$

$$(5.5) \quad -\Delta V = 4\pi(\nu_+^2 + \nu_-^2 - \rho_b),$$

in  $n\Gamma$  with periodic boundary condition. Note that the normalization constraint (5.2) is contained in (5.5) as the solvability condition. The potential  $V$  is determined up to a constant by (5.2), the constant is fixed by (5.3) and (5.4) through the solvability condition of (5.2).

For later use, let us also write down the Euler-Lagrange equations in  $\varepsilon$ -scaling, which is just a rescaling of (5.3)–(5.5).

$$(5.6) \quad -\varepsilon^2 \Delta \nu_+^\varepsilon + \frac{5}{3} (\nu_+^\varepsilon)^{7/3} - \frac{4}{3} (\nu_+^\varepsilon)^{5/3} + (V^\varepsilon - h) \nu_+^\varepsilon = 0;$$

$$(5.7) \quad -\varepsilon^2 \Delta \nu_-^\varepsilon + \frac{5}{3} (\nu_-^\varepsilon)^{7/3} - \frac{4}{3} (\nu_-^\varepsilon)^{5/3} + (V^\varepsilon + h) \nu_-^\varepsilon = 0;$$

$$(5.8) \quad -\varepsilon^2 \Delta V^\varepsilon = 4\pi((\nu_+^\varepsilon)^2 + (\nu_-^\varepsilon)^2 - \rho_b^\varepsilon),$$

in  $\Gamma$  with periodic boundary condition. We have the scaling relations

$$\nu_\pm^\varepsilon(x) = \nu_\pm(x/\varepsilon), \quad V^\varepsilon(x) = V(x/\varepsilon), \quad \rho_b^\varepsilon(x) = \rho_b(x/\varepsilon).$$

In analogy with the spirit of the Cauchy-Born rule for crystal lattices, we expect that the electronic structure around a point  $x_0$  to be approximately given

by the electronic structure of a crystal under constant applied potential with amplitude  $h(\varepsilon x_0)$ . As we have discussed in the last section, the electronic structure for the system with the constant applied potential is given by  $\nu_{\pm, \text{CB}}(\cdot; h(\varepsilon x_0))$  and  $V_{\text{CB}}(\cdot; h(\varepsilon x_0))$ . Therefore, the electronic structure constructed using the spirit of the Cauchy-Born rule is

$$(5.9) \quad \nu_{\pm}(x) = \nu_{\pm, \text{CB}}(x; h(\varepsilon x)), \quad V(x) = V_{\text{CB}}(x; h(\varepsilon x)).$$

One main result of this paper is that under the stability conditions, the electronic structure constructed by the Cauchy-Born rule gives a good approximation to a solution to the TFDW equation. In other words, one can find a solution to the TFDW equation that is close to the Cauchy-Born approximation.

**Theorem 2.** *Under Assumption A, there exist positive constants  $h_0$ ,  $\varepsilon_0$  and  $\delta$ , such that for any  $h \in C^\infty(\Gamma)$ ,  $\|h\|_{L^\infty(\Gamma)} \leq h_0$  and  $\varepsilon \leq \varepsilon_0$ , there exists a unique  $u = (\nu_+, \nu_-, V) \in (H_n^2)^3$ , with the properties*

- *$u$  is a solution to the Euler-Lagrange equation,*

$$\mathcal{F}(u) = 0;$$

- *$u$  is close to the approximation given by the Cauchy-Born rule*

$$\|u - u_{\text{CB}}(x; h(\varepsilon x))\|_{(H_n^2)^3} \leq \delta \varepsilon.$$

We notice that once the solution to the Euler-Lagrange equation is determined as  $u = (\nu_{\pm}, V)$ , the associated energy can be written as

$$\begin{aligned} I_n^h(\nu_+, \nu_-) &= \int_{n\Gamma} \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int_{n\Gamma} \nu_+^{8/3} + \nu_-^{8/3} \\ &\quad + \int_{n\Gamma} V(\rho - \rho_b) - \int_{n\Gamma} h(\varepsilon x)m. \end{aligned}$$

As a consequence of Theorem 2, the energy is well approximated by the Cauchy-Born rule, given by

$$(5.10) \quad I_{n, \text{CB}}^h = \int_{n\Gamma} E_{\text{CB}}(h(\varepsilon x)) \, dx = \frac{1}{\varepsilon^3} \int_{\Gamma} E_{\text{CB}}(h(x)) \, dx,$$

with  $E_{\text{CB}}$  defined by

$$\begin{aligned} (5.11) \quad E_{\text{CB}}(h) &= \oint_{\Gamma} \nu_{+, \text{CB}}^{10/3} + \nu_{-, \text{CB}}^{10/3} + |\nabla \nu_{+, \text{CB}}|^2 + |\nabla \nu_{-, \text{CB}}|^2 - \oint_{n\Gamma} \nu_{+, \text{CB}}^{8/3} + \nu_{-, \text{CB}}^{8/3} \\ &\quad + \oint_{\Gamma} V_{\text{CB}}(\rho_{\text{CB}} - \rho_b) - h \oint_{\Gamma} m_{\text{CB}}, \end{aligned}$$

where  $\nu_{\pm, \text{CB}} = \nu_{\pm, \text{CB}}(\cdot; h)$  and similarly for other terms. Note that, at least formally, we have

$$(5.12) \quad \int_{\Gamma} E_{\text{CB}}(h(x)) \, dx = \inf_m \left( \int_{\Gamma} \tilde{E}_{\text{CB}}(m(x)) - h(x)m(x) \, dx \right).$$

Here  $\tilde{E}_{\text{CB}}(m)$  is given by the cell problem

$$\tilde{E}_{\text{CB}}(m) = \inf_{\nu_{\pm}: m_{\text{tot}}=m} \left\{ \int_{\Gamma} \nu_+^{10/3} + \nu_-^{10/3} + |\nabla \nu_+|^2 + |\nabla \nu_-|^2 - \int_{\Gamma} \nu_+^{8/3} + \nu_-^{8/3} + \frac{1}{2|\Gamma|} D_{\Gamma}(\rho - \rho_b, \rho - \rho_b) \right\},$$

where  $m_{\text{tot}} = \int_{\Gamma} \nu_+^2 - \nu_-^2$  is constrained to be equal to  $m$ .

In terms of micromagnetics, the former term on the right hand side of (5.12) is the anisotropic term of magnetization, and the latter term is the energy due to external magnetic field. Compared with the usual energy functional used in micromagnetics [2, 3], we do not have the stray field energy term (the nonlocal term) for the magnetostatic interaction and the exchange term. The reason that the nonlocal term is missing is due to the fact that the Thomas-Fermi-Dirac-von Weizsäcker model only contains a local term of  $m$ . One can try to add a term that account for the magnetostatic interaction at the microscopic level, we would then obtain the nonlocal term in (5.12). However, this is only natural for a non-collinear model, which will be studied in future publications. The reason that we do not have the exchange term in the energy functional is more fundamental. Since the scaling we consider only covers the smooth regime, there is no hope on the leading order to recover the exchange term which penalize change of magnetization on the scale comparable to the atomic length scale. One might hope to obtain the exchange term by a different scaling limit or going to the next order, for example, zooming in the region of domain wall. We would not go further in this direction in the current work.

## 6. TWO SCALE ANALYSIS

**6.1. Matched asymptotics.** In this section, we use two scale analysis to build a high-order approximate solution to the Euler-Lagrange equation.

It is more convenient to work with  $\varepsilon$ -scaling in this section. The choice of scaling is also in agreement with standard homogenization problems. Let us recall the Euler-Lagrange equations under  $\varepsilon$ -scaling.

$$\begin{aligned} -\varepsilon^2 \Delta \nu_+^{\varepsilon} + \frac{5}{3}(\nu_+^{\varepsilon})^{7/3} - \frac{4}{3}(\nu_+^{\varepsilon})^{5/3} + (V^{\varepsilon} - h)\nu_+^{\varepsilon} &= 0; \\ -\varepsilon^2 \Delta \nu_-^{\varepsilon} + \frac{5}{3}(\nu_-^{\varepsilon})^{7/3} - \frac{4}{3}(\nu_-^{\varepsilon})^{5/3} + (V^{\varepsilon} + h)\nu_-^{\varepsilon} &= 0; \\ -\varepsilon^2 \Delta V^{\varepsilon} &= 4\pi((\nu_+^{\varepsilon})^2 + (\nu_-^{\varepsilon})^2 - \rho_b^{\varepsilon}). \end{aligned}$$

We take the following two-scale ansatz

$$\begin{aligned} \nu_+^{\varepsilon}(x) &= \nu_{+,0}(x, x/\varepsilon) + \varepsilon \nu_{+,1}(x, x/\varepsilon) + \varepsilon^2 \nu_{+,2}(x, x/\varepsilon); \\ \nu_-^{\varepsilon}(x) &= \nu_{-,0}(x, x/\varepsilon) + \varepsilon \nu_{-,1}(x, x/\varepsilon) + \varepsilon^2 \nu_{-,2}(x, x/\varepsilon); \\ V^{\varepsilon}(x) &= V_0(x, x/\varepsilon) + \varepsilon V_1(x, x/\varepsilon) + \varepsilon^2 V_2(x, x/\varepsilon). \end{aligned}$$

Substituting into the equations and matching orders, we obtain for the leading order

$$(6.1) \quad -\Delta_z \nu_{+,0}(x, z) + \frac{5}{3} \nu_{+,0}^{7/3}(x, z) - \frac{4}{3} \nu_{+,0}^{5/3}(x, z) + (V_0(x, z) - h(x)) \nu_{+,0}(x, z) = 0;$$

$$(6.2) \quad -\Delta_z \nu_{-,0}(x, z) + \frac{5}{3} \nu_{-,0}^{7/3}(x, z) - \frac{4}{3} \nu_{-,0}^{5/3}(x, z) + (V_0(x, z) + h(x)) \nu_{-,0}(x, z) = 0;$$

$$(6.3) \quad -\Delta_z V_0(x, z) = 4\pi(\nu_{+,0}^2(x, z) + \nu_{-,0}^2(x, z) - \rho_b(z)).$$

The solutions are given by

$$(6.4) \quad \nu_{+,0}(x, z) = \nu_{+,CB}(z; h(x)), \quad \nu_{-,0}(x, z) = \nu_{-,CB}(z; h(x)),$$

with the potential given by

$$(6.5) \quad V_0(x, z) = V_{CB}(z; h(x)).$$

The next order equations are given by

$$(6.6) \quad -\Delta_z \nu_{+,1} - 2\nabla_x \cdot \nabla_z \nu_{+,0} + \frac{35}{9} \nu_{+,0}^{4/3} \nu_{+,1} - \frac{20}{9} \nu_{+,0}^{2/3} \nu_{+,1} + (V_0 - h) \nu_{+,1} + V_1 \nu_{+,0} = 0;$$

$$(6.7) \quad -\Delta_z \nu_{-,1} - 2\nabla_x \cdot \nabla_z \nu_{-,0} + \frac{35}{9} \nu_{-,0}^{4/3} \nu_{-,1} - \frac{20}{9} \nu_{-,0}^{2/3} \nu_{-,1} + (V_0 + h) \nu_{-,1} + V_1 \nu_{-,0} = 0;$$

$$(6.8) \quad -\Delta_z V_1 - 2\nabla_x \cdot \nabla_z V_0 = 8\pi(\nu_{+,0} \nu_{+,1} + \nu_{-,0} \nu_{-,1}).$$

Using the linearized operator  $\mathcal{L}_h$ , we may rewrite the set of equations as

$$(6.9) \quad \mathcal{L}_h \begin{pmatrix} \nu_{+,1} \\ \nu_{-,1} \\ V_1 \end{pmatrix} = \begin{pmatrix} f_{+,1} \\ f_{-,1} \\ g_1 \end{pmatrix},$$

where

$$f_{+,1} = 2\nabla_x \cdot \nabla_z \nu_{+,0}; \quad f_{-,1} = 2\nabla_x \cdot \nabla_z \nu_{-,0}; \quad g_1 = -\frac{1}{4\pi} \nabla_x \cdot \nabla_z V_0.$$

By the regularity of  $\nu_{\pm,0}$  and  $V_0$ , it is easy to see that  $f_{\pm,1}, g_1 \in C^\infty(\Gamma, H_1^1)$ . Inverting  $\mathcal{L}_h$  by Proposition 4.1, we then obtain  $\nu_{\pm,1}$ ,  $V_1$ , and

$$\nu_{\pm,1} \in C^\infty(\Gamma, H_1^3) \quad V_1 \in C^\infty(\Gamma, H_1^3).$$



We also have the third order equations

$$(6.10) \quad -\Delta_z \nu_{+,2} - 2\nabla_x \cdot \nabla_z \nu_{+,1} - \Delta_x \nu_{+,0} + \frac{35}{9} \nu_{+,0}^{4/3} \nu_{+,2} + \frac{70}{27} \nu_{+,0}^{1/3} \nu_{+,1}^2 \\ - \frac{20}{9} \nu_{+,0}^{2/3} \nu_{+,2} - \frac{20}{27} \nu_{+,0}^{-1/3} \nu_{+,1}^2 + (V_0 - h) \nu_{+,2} + V_1 \nu_{+,1} + V_2 \nu_{+,0} = 0;$$

$$(6.11) \quad -\Delta_z \nu_{-,2} - 2\nabla_x \cdot \nabla_z \nu_{-,1} - \Delta_x \nu_{-,0} + \frac{35}{9} \nu_{-,0}^{4/3} \nu_{-,2} + \frac{70}{27} \nu_{-,0}^{1/3} \nu_{-,1}^2 \\ - \frac{20}{9} \nu_{-,0}^{2/3} \nu_{-,2} - \frac{20}{27} \nu_{-,0}^{-1/3} \nu_{-,1}^2 + (V_0 + h) \nu_{-,2} + V_1 \nu_{-,1} + V_2 \nu_{-,0} = 0;$$

$$(6.12) \quad -\Delta_z V_2 - 2\nabla_x \cdot \nabla_z V_1 - \Delta_x V_0 = 4\pi(\nu_{+,1}^2 + 2\nu_{+,0} \nu_{+,2} + \nu_{-,1}^2 + 2\nu_{-,0} \nu_{-,2}).$$

As the first order correction, we solve

$$(6.13) \quad \mathcal{L}_h \begin{pmatrix} \nu_{+,2} \\ \nu_{-,2} \\ V_2 \end{pmatrix} = \begin{pmatrix} f_{+,2} \\ f_{-,2} \\ g_2 \end{pmatrix},$$

where

$$f_{+,2} = 2\nabla_x \cdot \nabla_z \nu_{+,1} + \Delta_x \nu_{+,0} - \frac{70}{27} \nu_{+,0}^{1/3} \nu_{+,1}^2 + \frac{20}{27} \nu_{+,0}^{-1/3} \nu_{+,1}^2 - V_1 \nu_{+,1}; \\ f_{-,2} = 2\nabla_x \cdot \nabla_z \nu_{-,1} + \Delta_x \nu_{-,0} - \frac{70}{27} \nu_{-,0}^{1/3} \nu_{-,1}^2 + \frac{20}{27} \nu_{-,0}^{-1/3} \nu_{-,1}^2 - V_1 \nu_{-,1}; \\ g_2 = -\frac{1}{8\pi} (2\nabla_x \cdot \nabla_z V_1 + \Delta_x V_0) - \frac{1}{2} (\nu_{+,1}^2 + \nu_{-,1}^2).$$

Therefore, (6.13) is solvable to give  $\nu_{\pm,2}$  and  $V_2$  in  $C^\infty(\Gamma, H_1^3)$ .

This procedure can be carried on for even higher order terms. We omit the details here.

*Remark.* There is an important difference between the Thomas-Fermi type of models and the Kohn-Sham type of models considered in [5]. In the two scale analysis for the Kohn-Sham map developed in [5], the macroscopic part of the potential on the leading order depends on the density on the order of  $\varepsilon^2$ , making the closure a bit unusual. Here, the macroscopic part  $\langle V_0 \rangle$  is determined on the leading order, and it imposes a constraint on the third order densities. In particular, as observed in [4] and [8], the Coulomb potential in Thomas-Fermi type of models are determined locally to the leading order, while it is not the case for Kohn-Sham type of models. This also leads to important differences in developing multiscale algorithms for these two type of models.

**6.2. Approximate solution.** Let us take the approximate solution built in the last section:

$$\nu_+(x) = \nu_{+,0}(\varepsilon x, x) + \varepsilon \nu_{+,1}(\varepsilon x, x) + \varepsilon^2 \nu_{+,2}(\varepsilon x, x); \\ \nu_-(x) = \nu_{-,0}(\varepsilon x, x) + \varepsilon \nu_{-,1}(\varepsilon x, x) + \varepsilon^2 \nu_{-,2}(\varepsilon x, x); \\ V(x) = V_0(\varepsilon x, x) + \varepsilon V_1(\varepsilon x, x) + \varepsilon^2 V_2(\varepsilon x, x).$$

Here we have rescaled the functions into the units in which the lattice parameter is 1.

**Proposition 6.1.**

$$\|\mathcal{F}(\nu_+, \nu_-, V)\|_{(L_n^2)^3} \lesssim \varepsilon^3.$$

*Proof.* Denote

$$(f_+, f_-, g) = \mathcal{F}(\nu_+, \nu_-, V).$$

We write

$$\begin{aligned} (6.14) \quad f_+ &= -\Delta \nu_+^\varepsilon + \frac{5}{3}(\nu_+^\varepsilon)^{7/3} - \frac{4}{3}(\nu_+^\varepsilon)^{5/3} + (V^\varepsilon - h)\nu_+^\varepsilon \\ &= f_{+,1} + f_{+,2} + f_{+,3} + f_{+,4}, \end{aligned}$$

where we have introduced the shorthand notation

$$\begin{aligned} f_{+,1} &= -\varepsilon^3 \Delta_x \nu_{+,1} - 2\varepsilon^3 \nabla_x \cdot \nabla_z \nu_{+,2} - \varepsilon^4 \Delta_x \nu_{+,2}; \\ f_{+,2} &= \frac{5}{3}(\nu_{+,0} + \varepsilon \nu_{+,1} + \varepsilon^2 \nu_{+,2})^{7/3} - \frac{5}{3}\nu_{+,0}^{7/3} \\ &\quad - \frac{35}{9}\varepsilon \nu_{+,0}^{4/3}(\nu_{+,1} + \varepsilon \nu_{+,2}) - \frac{70}{27}\varepsilon^2 \nu_{+,0}^{1/3} \nu_{+,1}^2; \\ f_{+,3} &= -\frac{4}{3}(\nu_{+,0} + \varepsilon \nu_{+,1} + \varepsilon^2 \nu_{+,2})^{5/3} + \frac{4}{3}\nu_{+,0}^{5/3} \\ &\quad + \frac{20}{9}\varepsilon \nu_{+,0}^{2/3}(\nu_{+,1} + \varepsilon \nu_{+,2}) + \frac{20}{27}\varepsilon^2 \nu_{+,0}^{-1/3} \nu_{+,1}^2; \\ f_{+,4} &= \varepsilon^3 V_1 \nu_{+,2} + \varepsilon^3 V_2 \nu_{+,1} + \varepsilon^4 V_2 \nu_{+,2}. \end{aligned}$$

Here  $\nu$  and  $V$  are evaluated at  $(\varepsilon x, x)$ . Since  $\|f\|_{L_n^2} \leq \|f\|_{L_n^\infty}$ , it suffices to prove that  $\|f_{+,i}\|_{L_n^\infty} \lesssim \varepsilon^3$  for  $i = 1, 2, 3, 4$ . Since we have  $\nu_{+,1}, \nu_{+,2} \in C^\infty(\Gamma, H_1^3)$ , by Sobolev embedding  $H_1^2 \subset L^\infty(\Gamma)$ , it is easy to see that  $\|f_{+,1}\|_{L_n^\infty} \lesssim \varepsilon^3$ . The estimates for  $f_{+,2}$  and  $f_{+,3}$  follow from Taylor expansion. Finally, the desired estimate of  $f_{+,4}$  is obtained from Sobolev embedding applied on  $V_1, V_2, \nu_{+,1}$  and  $\nu_{+,2}$ . In summary, we have

$$\|f_+\|_{L_n^2} \lesssim \varepsilon^3.$$

The argument for  $f_-$  is completely the same as that for  $f_+$ . Let us consider

$$\begin{aligned} (6.15) \quad g &= -\varepsilon^2 \Delta V^\varepsilon - 4\pi((\nu_+^\varepsilon)^2 + (\nu_-^\varepsilon)^2 - \rho_b^\varepsilon) \\ &= g_1 + g_2 + g_3, \end{aligned}$$

where we have introduced the shorthands

$$\begin{aligned} g_1 &= -\varepsilon^3 \Delta_x V_1 - 2\varepsilon^3 \nabla_x \cdot \nabla_z V_2 - \varepsilon^4 \Delta_x V_2; \\ g_2 &= 8\pi \varepsilon^3 \nu_{+,1} \nu_{+,2} + 4\pi \varepsilon^4 \nu_{+,2}^2; \\ g_3 &= 8\pi \varepsilon^3 \nu_{-,1} \nu_{-,2} + 4\pi \varepsilon^4 \nu_{-,2}^2. \end{aligned}$$

It is clear that by analogous argument as above, we have the estimate  $\|g\|_{L_n^2} \lesssim \varepsilon^3$ .  $\square$

## 7. PROOF OF THEOREM 2

Similar to [5, 6], we use Newton-Raphson iteration to find a solution to the Euler-Lagrange equation in the neighborhood of the approximated solution constructed above.

We will start with the approximate solution we constructed

$$(7.1) \quad u^0 = (\nu_+^0, \nu_-^0, V^0) \in \mathcal{D}_n,$$

where

$$\begin{aligned} \nu_+^0(x) &= \nu_{+,0}(\varepsilon x, x) + \varepsilon \nu_{+,1}(\varepsilon x, x) + \varepsilon^2 \nu_{+,2}(\varepsilon x, x); \\ \nu_-^0(x) &= \nu_{-,0}(\varepsilon x, x) + \varepsilon \nu_{-,1}(\varepsilon x, x) + \varepsilon^2 \nu_{-,2}(\varepsilon x, x); \\ V^0(x) &= V_0(\varepsilon x, x) + \varepsilon V_1(\varepsilon x, x) + \varepsilon^2 V_2(\varepsilon x, x). \end{aligned}$$

Here the superscript 0 is used to indicate the initial point for the Newton iteration. Note that we have rescaled the functions, so that  $\nu_\pm^0$  and  $V^0$  are defined in  $n\Gamma$ .

We need several additional lemmas for the proof of Theorem 2. The following lemmas are proved under the assumptions in the statement of Theorem 2.

**Lemma 7.1.** *For any  $\kappa > 0$ , there exists positive constants  $h_0$  and  $\varepsilon_0$ , such that for all  $\varepsilon \leq \varepsilon_0$  and  $h$  with  $\|h\|_{L^\infty(\Gamma)} \leq h_0$ , we have*

$$\|\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}\|_{\mathcal{L}((L_n^2)^3)} \leq \kappa.$$

*Proof.* By definition, given  $(\omega_+, \omega_-, W) \in (H_n^2)^3$ , we have

$$(7.2) \quad (\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}) \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix} = \begin{pmatrix} \delta\mathcal{L}_+ & 0 & \delta\nu_+ \\ 0 & \delta\mathcal{L}_- & \delta\nu_- \\ \delta\nu_+ & \delta\nu_- & 0 \end{pmatrix} \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix} \equiv \begin{pmatrix} f_+ \\ f_- \\ g \end{pmatrix},$$

where the last equality serves as a definition and we have introduced the notations

$$\begin{aligned} \delta\mathcal{L}_+ &= \frac{35}{9} \left( (\nu_+^0)^{4/3} - \nu_{+, \text{per}}^{4/3} \right) - \frac{20}{9} \left( (\nu_+^0)^{2/3} - \nu_{+, \text{per}}^{2/3} \right) + (V^0 - h - V_{\text{per}}), \\ \delta\mathcal{L}_- &= \frac{35}{9} \left( (\nu_-^0)^{4/3} - \nu_{-, \text{per}}^{4/3} \right) - \frac{20}{9} \left( (\nu_-^0)^{2/3} - \nu_{-, \text{per}}^{2/3} \right) + (V^0 + h - V_{\text{per}}), \end{aligned}$$

and

$$\delta\nu_\pm = \nu_\pm^0 - \nu_{\pm, \text{per}}.$$

Note that

$$\begin{aligned} \delta\nu_+(x) &= \nu_{+,0}(\varepsilon x, x) + \varepsilon \nu_{+,1}(\varepsilon x, x) + \varepsilon^2 \nu_{+,2}(\varepsilon x, x) - \nu_{+, \text{per}}(x) \\ &= (\nu_{+, \text{CB}}(x; h(\varepsilon x)) - \nu_{+, \text{CB}}(x; 0)) + \varepsilon \nu_{+,1}(\varepsilon x, x) + \varepsilon^2 \nu_{+,2}(\varepsilon x, x). \end{aligned}$$

By the smooth dependence on  $\nu_{+, \text{CB}}(\cdot; h)$  on the parameter  $h$ , we have

$$\|\nu_{+, \text{CB}}(x; h(\varepsilon x)) - \nu_{+, \text{CB}}(x; 0)\|_{L^\infty(n\Gamma)} \lesssim \|h\|_{L^\infty(\Gamma)}.$$

The other two terms are of higher order in  $\varepsilon$ , since  $\nu_{+,1}(\varepsilon x, x)$  and  $\nu_{+,2}(\varepsilon x, x)$  are bounded uniformly in  $n\Gamma$ . Therefore, we obtain

$$\|\delta\nu_+\|_{L^\infty(n\Gamma)} \lesssim \|h\|_{L^\infty(\Gamma)} + \varepsilon.$$

Obviously, the same estimates also hold for  $\delta\nu_-$ . Hence,

$$\begin{aligned} \|g\|_{L_n^2} &\leq \|\delta\nu_+\|_{L^\infty(n\Gamma)} \|\omega_+\|_{L_n^2} + \|\delta\nu_-\|_{L^\infty(n\Gamma)} \|\omega_-\|_{L_n^2} \\ &\lesssim (\|h\|_{L^\infty(\Gamma)} + \varepsilon) (\|\omega_+\|_{L_n^2} + \|\omega_-\|_{L_n^2}). \end{aligned}$$

The analysis for  $f_+$  and  $f_-$  are the same, let us study  $f_+$ . Using Taylor expansion, we have

$$\left| (\nu_+^0)^{4/3}(x) - (\nu_{+, \text{per}})^{4/3}(x) \right| \leq \frac{4}{3} \left| \nu_+^0(x) - \nu_{+, \text{per}}(x) \right| \max_{\nu \in [\nu_{+, \min}(x), \nu_{+, \max}(x)]} \nu^{1/3},$$

where  $\nu_{+, \min}(x) = \min(\nu_+^0(x), \nu_{+, \text{per}}(x))$  and  $\nu_{+, \max}(x) = \max(\nu_+^0(x), \nu_{+, \text{per}}(x))$ . Since

$$|\nu_+^0(x) - \nu_{+, \text{per}}(x)| \leq \|\delta\nu_+\|_{L^\infty} \lesssim \|h\|_{L^\infty(\Gamma)} + \varepsilon,$$

we have for  $h_0$  and  $\varepsilon_0$  sufficiently small,  $\nu_+^0(x)$  is bounded from above and also from below away from zero uniformly for  $x \in n\Gamma$ . Hence  $\max_{\nu \in [\nu_{+, \min}(x), \nu_{+, \max}(x)]} \nu^{1/3}$  is bounded. Therefore,

$$\left| (\nu_+^0)^{4/3}(x) - (\nu_{+, \text{per}})^{4/3}(x) \right| \lesssim \|h\|_{L^\infty(\Gamma)} + \varepsilon.$$

It follows that

$$(7.3) \quad \left\| \frac{35}{9} ((\nu_+^0)^{4/3} - (\nu_{+, \text{per}})^{4/3}) \omega_+ \right\|_{L_n^2} \lesssim (\|h\|_{L^\infty(\Gamma)} + \varepsilon) \|\omega_+\|_{L_n^2}.$$

Using similar arguments, we have

$$(7.4) \quad \left\| \frac{20}{9} ((\nu_+^0)^{2/3} - (\nu_{+, \text{per}})^{2/3}) \omega_+ \right\|_{L_n^2} \lesssim (\|h\|_{L^\infty(\Gamma)} + \varepsilon) \|\omega_+\|_{L_n^2}.$$

Compare the difference of  $V^0$  and  $V_{\text{per}}$ , we have

$$V^0 - V_{\text{per}} = V_{\text{CB}}(x; h(\varepsilon x)) - V_{\text{CB}}(x; 0) + \varepsilon V_1(\varepsilon x, x) + \varepsilon^2 V_2(\varepsilon x, x).$$

Analogous to the control of  $\delta\nu_+$ , we have

$$\|V^0 - V_{\text{per}}\|_{L^\infty(n\Gamma)} \lesssim \|h\|_{L^\infty(\Gamma)} + \varepsilon.$$

Therefore,

$$(7.5) \quad \begin{aligned} \|(V^0 - H - V_{\text{per}}) \omega_+\|_{L_n^2} &\leq \|V^0 - h - V_{\text{per}}\|_{L^\infty(n\Gamma)} \|\omega_+\|_{L_n^2} \\ &\lesssim (\|h\|_{L^\infty(\Gamma)} + \varepsilon) \|\omega_+\|_{L_n^2}. \end{aligned}$$

We also have

$$(7.6) \quad \|\delta\nu_+ W\|_{L_n^2} \leq \|\delta\nu_+\|_{L^\infty(n\Gamma)} \|W\|_{L_n^2} \lesssim (\|h\|_{L^\infty(\Gamma)} + \varepsilon) \|W\|_{L_n^2}.$$

Combining (7.3)–(7.6), we obtain

$$\|f_+\|_{L_n^2} \lesssim (\|h\|_{L^\infty(\Gamma)} + \varepsilon) (\|\omega_+\|_{L_n^2} + \|W\|_{L_n^2}).$$

Therefore,

$$\|\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}\|_{\mathcal{L}((L_n^2)^3)} \lesssim \|h\|_{L^\infty(\Gamma)} + \varepsilon.$$

The conclusion of the Lemma follows.  $\square$

**Corollary 7.2.** *There exists positive constants  $h_0$  and  $\varepsilon_0$ , such that for all  $\varepsilon \leq \varepsilon_0$  and  $h$  with  $\|h\|_{L^\infty(\Gamma)} \leq h_0$ , we have*

$$\|\mathcal{L}_{u^0}^{-1}\|_{\mathcal{L}((L_n^2)^3, (H_n^2)^3)} \lesssim 1.$$

*In particular, the bound is independent of  $n$ .*

*Proof.* Since

$$\mathcal{L}_{u^0} = \mathcal{L}_{\text{per}} + (\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}),$$

we have

$$\mathcal{L}_{u^0}^{-1} = \mathcal{L}_{\text{per}}^{-1} (\mathcal{I} + (\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}) \mathcal{L}_{\text{per}}^{-1})^{-1}$$

if the right hand side is well-defined, where  $\mathcal{I}$  is the identity operator.

By Assumption A, there exists  $\kappa > 0$  such that  $\|\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}\|_{\mathcal{L}((H_n^2)^3, (L_n^2)^3)} \leq \kappa$  implies

$$\|(\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}) \mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((H_n^2)^3)} \leq 1/2,$$

and hence  $\mathcal{I} + (\mathcal{L}_{u^0} - \mathcal{L}_{\text{per}}) \mathcal{L}_{\text{per}}^{-1}$  is invertible on  $(H_n^2)^3$  with the norm of the inverse less than 2. Therefore, by Lemma 7.1, there exists  $h_0$  and  $\varepsilon_0$  sufficiently small that

$$\|\mathcal{L}_{u^0}^{-1}\|_{\mathcal{L}((L_n^2)^3, (H_n^2)^3)} \leq 2 \|\mathcal{L}_{\text{per}}^{-1}\|_{\mathcal{L}((L_n^2)^3, (H_n^2)^3)}.$$

The corollary is proved by combining the above inequality with Assumption A.  $\square$

**Lemma 7.3.** *If  $u, u'$  satisfy  $\|u - u^0\|_{(H_n^2)^3} \leq \gamma \varepsilon^3$ ,  $\|u' - u^0\|_{(H_n^2)^3} \leq \gamma \varepsilon^3$ , then*

$$\|\mathcal{L}_u - \mathcal{L}_{u'}\|_{\mathcal{L}((L_n^2)^3)} \lesssim C(\gamma) \varepsilon^{-3/2} \|u - u'\|_{(H_n^2)^3}.$$

*Proof.* By definition, given  $(\omega_+, \omega_-, W) \in (L_n^2)^3$ , we have

$$(7.7) \quad (\mathcal{L}_u - \mathcal{L}_{u'}) \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix} = \begin{pmatrix} \delta \mathcal{L}_+ & 0 & \delta \nu_+ \\ 0 & \delta \mathcal{L}_- & \delta \nu_- \\ \delta \nu_+ & \delta \nu_- & 0 \end{pmatrix} \begin{pmatrix} \omega_+ \\ \omega_- \\ W \end{pmatrix} \equiv \begin{pmatrix} f_+ \\ f_- \\ g \end{pmatrix},$$

where the last equality serves as a definition and we have introduced the notations

$$\delta \mathcal{L}_\pm = \frac{35}{9} \left( (\nu_\pm)^{4/3} - (\nu'_\pm)^{4/3} \right) - \frac{20}{9} \left( (\nu_\pm)^{2/3} - (\nu'_\pm)^{2/3} \right) + (V - V'),$$

and

$$\delta \nu_\pm = \nu_\pm - \nu'_\pm.$$

First let us control  $g$ . By Sobolev inequality, we have

$$\|\delta \nu_\pm\|_{L^\infty(n\Gamma)} \lesssim \|\delta \nu_\pm\|_{H^2(n\Gamma)} = n^{3/2} \|\delta \nu_\pm\|_{H_n^2}.$$

Hence,

$$\begin{aligned} \|g\|_{L_n^2} &= \|\delta\nu_+\omega_+ + \delta\nu_-\omega_-\|_{L_n^2} \\ &\leq \|\delta\nu_+\|_{L^\infty(n\Gamma)}\|\omega_+\|_{L_n^2} + \|\delta\nu_-\|_{L^\infty(n\Gamma)}\|\omega_-\|_{L_n^2} \\ &\leq n^{3/2}\left(\|\delta\nu_+\|_{H_n^2}\|\omega_+\|_{L_n^2} + \|\delta\nu_-\|_{H_n^2}\|\omega_-\|_{L_n^2}\right). \end{aligned}$$

Similarly, we have

$$\|\delta\nu_+W\|_{L_n^2} \leq n^{3/2}\|\delta\nu_+\|_{H_n^2}\|W\|_{L_n^2}.$$

Now consider the term  $\delta\mathcal{L}_+\omega_+$ , we have

$$|(\nu_+)^{4/3}(x) - (\nu'_+)^{4/3}(x)| \leq \frac{4}{3}|\nu_+(x) - \nu'_+(x)| \max_{\nu \in [\nu_{+, \min}(x), \nu_{+, \max}(x)]} \nu^{1/3},$$

where  $\nu_{+, \min}(x) = \min(\nu_+(x), \nu'_+(x))$  and  $\nu_{+, \max}(x) = \max(\nu_+(x), \nu'_+(x))$ . Since

$$|\nu_+(x) - \nu'_+(x)| \leq \|\nu_+ - \nu'_+\|_{L^\infty} \lesssim n^{3/2}\|\nu_+ - \nu'_+\|_{H_n^2} \leq \gamma\varepsilon^{3/2},$$

we have for  $\varepsilon$  sufficiently small,  $\nu_+(x)$  is bounded from above and also from below away from zero uniformly for  $x \in n\Gamma$ . The same holds for  $\nu'_+(x)$ , and hence  $\max_{\nu \in [\nu_{+, \min}(x), \nu_{+, \max}(x)]} \nu^{1/3}$  is bounded. Therefore,

$$|(\nu_+)^{4/3}(x) - (\nu'_+)^{4/3}(x)| \lesssim C(\gamma)|\nu_+(x) - \nu'_+(x)| \lesssim C(\gamma)n^{3/2}\|\nu_+ - \nu'_+\|_{H_n^2}.$$

It follows that

$$\left\| \frac{35}{9}((\nu_+)^{4/3} - (\nu'_+)^{4/3})\omega_+ \right\|_{L_n^2} \lesssim C(\gamma)n^{3/2}\|\nu_+ - \nu'_+\|_{H_n^2}\|\omega_+\|_{L_n^2}.$$

The argument for the remaining two terms in  $\delta\mathcal{L}_+\omega_+$  is similar, and we conclude that

$$\|\delta\mathcal{L}_+\omega_+\|_{L_n^2} \lesssim C(\gamma)n^{3/2}\|u - u'\|_{(H_n^2)^3}\|\omega_+\|_{L_n^2},$$

and analogously

$$\|\delta\mathcal{L}_-\omega_-\|_{L_n^2} \lesssim C(\gamma)n^{3/2}\|u - u'\|_{(H_n^2)^3}\|\omega_-\|_{L_n^2}.$$

In summary, we have  $\|\delta\mathcal{L}\|_{\mathcal{L}((L_n^2)^3)} \lesssim C(\gamma)n^{3/2}\|u - u'\|_{(H_n^2)^3} = C(\gamma)\varepsilon^{-3/2}\|u - u'\|_{(H_n^2)^3}$ .  $\square$

**Lemma 7.4.** *If  $u, u'$  satisfy  $\|u - u^0\|_{(H_n^2)^3} \leq \gamma\varepsilon^3$ ,  $\|u' - u^0\|_{(H_n^2)^3} \leq \gamma\varepsilon^3$ , then*

$$\|\mathcal{L}_{u^0}^{-1}(\mathcal{F}(u) - \mathcal{F}(u') - \mathcal{L}_{u^0}(u - u'))\|_{(H_n^2)^3} \lesssim C(\gamma)\varepsilon^{3/2}\|u - u'\|_{(H_n^2)^3}.$$

*Proof.* We write

$$\mathcal{F}(u) - \mathcal{F}(u') - \mathcal{L}_{u^0}(u - u') = \int_0^1 (\mathcal{L}_{u_t} - \mathcal{L}_{u^0})(u - u') dt,$$

where  $u_t = tu + (1-t)u'$ . It is easy to see that for any  $t \in [0, 1]$ , we have

$$\|u_t - u^0\|_{(H_n^2)^3} \leq \max\left(\|u - u^0\|_{(H_n^2)^3}, \|u' - u^0\|_{(H_n^2)^3}\right).$$

Therefore, using Lemma 7.3, we obtain

$$\begin{aligned} \|\mathcal{F}(u) - \mathcal{F}(u') - \mathcal{L}_{u^0}(u - u')\|_{(L_n^2)^3} &\leq \sup_{t \in [0,1]} \|\mathcal{L}_{u_t} - \mathcal{L}_{u^0}\|_{\mathcal{L}((L_n^2)^3)} \|u - u'\|_{(L_n^2)^3} \\ &\lesssim \varepsilon^{-3/2} C(\gamma) \sup_{t \in [0,1]} \|u_t - u^0\|_{(H_n^2)^3} \|u - u'\|_{(L_n^2)^3} \\ &\leq C(\gamma) \varepsilon^{3/2} \|u - u'\|_{(L_n^2)^3}. \end{aligned}$$

We conclude using Corollary 7.2.  $\square$

Now we are ready to prove the main result. We will actually prove a stronger version of Theorem 2 with higher order error estimate. Theorem 2 is clearly a corollary of the following result.

**Theorem 2'.** *Under the same assumptions as Theorem 2, there exists a unique  $u = (\nu_+, \nu_-, V) \in (H_n^2)^3$  such that*

- *$u$  is a solution to the Euler-Lagrange equation,*

$$\mathcal{F}(u) = 0;$$

- *$u$  is close to  $u^0$*

$$\|u - u^0\|_{(H_n^2)^3} \leq \delta \varepsilon^3.$$

*Proof.* Consider the nonlinear iteration

$$(7.8) \quad u^{k+1} = u^k - \mathcal{L}_{u^0}^{-1} \mathcal{F}(u^k),$$

with initial condition  $u^0$  given in (7.1).

Consider the first iteration ( $k = 0$  in (7.8)), we get

$$\|u^1 - u^0\|_{(H_n^2)^3} = \|\mathcal{L}_{u^0}^{-1} \mathcal{F}(u^0)\|_{(H_n^2)^3} \leq \|\mathcal{L}_{u^0}^{-1}\|_{\mathcal{L}((L_n^2)^3, (H_n^2)^3)} \|\mathcal{F}(u^0)\|_{(L_n^2)^3}.$$

By Proposition 6.1 and Corollary 7.2, there exists constant  $C_1$  such that

$$\|u^1 - u^0\|_{(H_n^2)^3} \leq C_1 \varepsilon^3 / 2.$$

Suppose we have proved for all  $k \leq k_0$ ,

$$(7.9) \quad \|u^k - u^0\|_{(H_n^2)^3} \leq C_1 \varepsilon^3,$$

by the iteration scheme (7.8), we have for all  $k \leq k_0$ ,

$$\begin{aligned} u^{k+1} - u^k &= u^k - u^{k-1} - \mathcal{L}_{u^0}^{-1} (\mathcal{F}(u^k) - \mathcal{F}(u^{k-1})) \\ &= -\mathcal{L}_{u^0}^{-1} (\mathcal{F}(u^k) - \mathcal{F}(u^{k-1}) - \mathcal{L}_{u^0}(u^k - u^{k-1})). \end{aligned}$$

Hence, by (7.9) and Lemma 7.4,

$$\|u^{k+1} - u^k\|_{(H_n^2)^3} \lesssim C(C_1) \varepsilon^{3/2} \|u^k - u^{k-1}\|_{(H_n^2)^3}.$$

For  $\varepsilon$  sufficiently small so that  $C(C_1) \varepsilon^{3/2} < 1/2$ , we then have

$$\|u^{k_0+1} - u^0\|_{(H_n^2)^3} \leq \sum_{k=0}^{k_0} \|u^{k+1} - u^k\|_{(H_n^2)^3} \leq 2 \|u^1 - u^0\|_{(H_n^2)^3} \leq C_1 \varepsilon^3.$$

Therefore, by induction, we have for all  $k \geq 0$ ,

$$\|u^k - u^0\|_{(H_n^2)^3} \leq C_1 \varepsilon^3,$$

and

$$(7.10) \quad \|u^{k+1} - u^k\|_{(H_n^2)^3} \leq \frac{1}{2} \|u^k - u^{k-1}\|_{(H_n^2)^3}.$$

Because of (7.10), the iteration converges to  $u^*$  and

$$\mathcal{F}(u^*) = 0.$$

In addition, we have

$$\|u^* - u^0\|_{(H_n^2)^3} \leq C_1 \varepsilon^3.$$

The local uniqueness also follows easily from (7.10).  $\square$

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